

10/717,958

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FILE 'HOME' ENTERED AT 16:22:25 ON 15 MAR 2005

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STRUCTURE FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7
DICTIONARY FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

```
=>  
Uploading C:\Program Files\Stnexp\Queries\107179581.str
```

L1 STRUCTURE UPLOADED

=> s 11
SAMPLE SEARCH INITIATED 16:22:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 350 TO ITERATE

100.0% PROCESSED 350 ITERATIONS 8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 5878 TO 8122
PROJECTED ANSWERS: 8. TO 329

L2 8 SEA SSS SAM L1

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=> s 11 ful
FULL SEARCH INITIATED 16:23:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7356 TO ITERATE

100.0% PROCESSED 7356 ITERATIONS
SEARCH TIME: 00.00.01

124 ANSWERS

L3 124 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 16:23:13 ON 15 MAR 2005
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FILE COVERS 1907 - 15 Mar 2005 VOL 142 ISS 12
FILE LAST UPDATED: 14 Mar 2005 (20050314/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 19 L3

=> s 14 and (process or making or make or made or prepar? or synthe?)
2060830 PROCESS
1374299 PROCESSES
3065131 PROCESS
(PROCESS OR PROCESSES)
244396 MAKING
30 MAKINGS
244420 MAKING
(MAKING OR MAKINGS)
205723 MAKE
158981 MAKES
354430 MAKE
(MAKE OR MAKES)
1138680 MADE
23 MADES
1138700 MADE
(MADE OR MADES)
1534101 PREPAR?
115055 PREP

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2025 PREPS
116881 PREP
(PREP OR PREPS)
1918786 PREPD
21 PREPDS
1918801 PREPD
(PREPD OR PREPDS)
106004 PREPG
12 PREPGS
106015 PREPG
(PREPG OR PREPGS)
2557303 PREPN
198667 PREPNS
2707792 PREPN
(PREPN OR PREPNS)
4488110 PREPAR?
(PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)
1433499 SYNTHES?
L5 9 L4 AND (PROCESS OR MAKING OR MAKE OR MADE OR PREPAR? OR SYNTHES?
)

=> d 15 ibib hitstr abs 1-9

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:567636 CAPLUS
DOCUMENT NUMBER: 141:290174
TITLE: Structural Bioinformatics and QSAR Analysis Applied to
the Acetylcholinesterase and Bispyridinium Aldoximes
AUTHOR(S): Mager, Peter; Weber, Anje
CORPORATE SOURCE: Research Group of Pharmacochemistry, Institute of
Pharmacology and Toxicology, Univ. Leipzig, Saxony,
Germany
SOURCE: Drug Design and Discovery (2003), 18(4), 127-150
CODEN: DDDIEV; ISSN: 1055-9612
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 84871-04-5
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)
(QSAR anal. applied to acetylcholinesterase and bispyridinium aldoximes
for qual. structural requirements for reactivating activity against
organophosphorus agents)
RN 84871-04-5 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[[[4-[(hydroxyimino)methyl]pyridinio]methoxy]methyl]- (9CI) (CA INDEX NAME)

/ Structure 1 in file .gra /

AB The methods of bioinformatics, mol. modeling, and quant.
structure-activity relationships (QSARs) using regression and artificial
neural network (ANN) analyses were applied to develop safer aldoxime
antidotes against poisoning by organophosphorus (OP) agents with high,
mean, and low aging rates. We start here from a mol. modeling of the
mouse AChE at an atomistic level. Aim is to predict qual. the structural
requirements of an aldoxime that shows an unique reactivating activity
against the three classes of OPs. An antidotal action should occur by a
three-site mechanism: the aldoxime groups of the first pyridinium ring
should point towards the catalytic site, and the second pyridinium ring

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and its substituents should be anchored at the peripheral and anionic subsites. Based on this model, it is predicted that a suitable substituent is based on an arginine-like moiety. Then, an ANN-based QSAR anal. using a training set of aldoximes with known structure and activities was applied. Its input layer consisted of seven nodes: the group-membership descriptors that parameterize the type of the OP, the logarithms of the distribution coeffs. at pH 7.4 and their squared term, the LUMO energies, the scaled molar refractions of the substituents, and their squared term. It was shown that the qual. prediction made by mol. modeling can be quantified by an ANN prediction.

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:258121 CAPLUS
DOCUMENT NUMBER: 140:425258
TITLE: *Synthesis and Aqueous Ozonation of Some Pyridinium Salts with Alkoxyethyl and Alkylthiomethyl Hydrophobic Groups*
AUTHOR(S): Pernak, Juliusz; Branicka, Monika
CORPORATE SOURCE: Institute of Chemical Technology and Engineering,
Poznan University of Technology, Poznan, 60-965, Pol.
SOURCE: Industrial & Engineering Chemistry Research (2004),
43(9), 1966-1974
CODEN: IECRED; ISSN: 0888-5885
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 571205-42-0P 571205-43-1P 571205-44-2P
571205-45-3P 571205-46-4P 571205-47-5P
571205-48-6P 571205-49-7P 571205-50-0P
RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and aqueous ozonation of some pyridinium salts with alkoxyethyl and alkylthiomethyl hydrophobic groups)
RN 571205-42-0 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(heptyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 2 in file .gra /

RN 571205-43-1 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(octyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 3 in file .gra /

RN 571205-44-2 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 4 in file .gra /

RN 571205-45-3 CAPLUS
CN Pyridinium, 1-[(decyloxy)methyl]-3-(dimethylamino)-, chloride (9CI) (CA INDEX NAME)

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/ Structure 5 in file .gra /

RN 571205-46-4 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 6 in file .gra /

RN 571205-47-5 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 7 in file .gra /

RN 571205-48-6 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(tetradecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 8 in file .gra /

RN 571205-49-7 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(hexadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 9 in file .gra /

RN 571205-50-0 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(octadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 10 in file .gra /

AB The reaction of ozone with a number of pyridinium salts containing 1-alkoxymethyl and 1-alkylthiomethyl substituents was determined at a total substrate concentration of 2 g/L. Ozonation of pyridinium salts was strongly dependent on the kinds and positions of the substituents in the pyridine ring. The most favorable were the third position and the substituents including hydroxyl or dimethylamino groups. In an aqueous solution, 1-(alkoxymethyl)-3-hydroxypyridinium, 1-(alkylthiomethyl)-3-hydroxypyridinium, and 1-(alkoxymethyl)-3-(dimethylamino)pyridinium salts reacted with ozone. The reaction was fast, and pyridinium salts were quant. removed. 1-(Alkoxyethyl)- and 1-(alkylthiomethyl)pyridinium chlorides were obtained by the Menschutkin reaction. In general, the procedure was simple and the reaction was productive and short. During the course of this study, we synthesized a new generation of cationic surfactants that were extremely reactive with ozone in an aqueous solution
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:346161 CAPLUS
DOCUMENT NUMBER: 139:149500

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TITLE: The properties of 1-alkoxymethyl-3-hydroxypyridinium and 1-alkoxymethyl-3-dimethylaminopyridinium chlorides
AUTHOR(S): Pernak, Juliusz; Branicka, Monika
CORPORATE SOURCE: Department of Chemical Technology, Poznan University of Technology, Poznan, 60-965, Pol.
SOURCE: Journal of Surfactants and Detergents (2003), 6(2), 119-123
CODEN: JSDEFL; ISSN: 1097-3958
PUBLISHER: AOCS Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:149500
IT 571205-38-4P 571205-39-5P 571205-40-8P
571205-41-9P 571205-42-0P 571205-43-1P
571205-44-2P 571205-45-3P 571205-46-4P
571205-47-5P 571205-48-6P 571205-49-7P
571205-50-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)
(preps. and antimicrobial activities of 1-alkoxymethyl-3-
substituted pyridinium chlorides)
RN 571205-38-4 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-(propoxymethyl)-, chloride (9CI) (CA INDEX NAME)

/ Structure 11 in file .gra /

RN 571205-39-5 CAPLUS
CN Pyridinium, 1-(butoxymethyl)-3-(dimethylamino)-, chloride (9CI) (CA INDEX NAME)

/ Structure 12 in file .gra /

RN 571205-40-8 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(pentyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 13 in file .gra /

RN 571205-41-9 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(hexyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 14 in file .gra /

RN 571205-42-0 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(heptyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 15 in file .gra /

RN 571205-43-1 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(octyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

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/ Structure 16 in file .gra /

RN 571205-44-2 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 17 in file .gra /

RN 571205-45-3 CAPLUS
CN Pyridinium, 1-[(decyloxy)methyl]-3-(dimethylamino)-, chloride (9CI) (CA INDEX NAME)

/ Structure 18 in file .gra /

RN 571205-46-4 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 19 in file .gra /

RN 571205-47-5 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 20 in file .gra /

RN 571205-48-6 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(tetradecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 21 in file .gra /

RN 571205-49-7 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(hexadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 22 in file .gra /

RN 571205-50-0 CAPLUS
CN Pyridinium, 3-(dimethylamino)-1-[(octadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 23 in file .gra /

AB Several 1-alkoxymethyl-3-substituted-pyridinium chlorides with alkoxy chains including from 3 to 18 carbon atoms were prepared by the reaction of 3-substituted-pyridine with chloromethyl alkyl ethers. The prepared chlorides were examined for their antielectrostatic effects and their antimicrobial activities. 1-Dodecyloxymethyl-3-dimethylaminopyridinium chloride (23) exhibited strong antimicrobial activity and a wide antimicrobial spectrum, similar to the activity of benzalkonium chloride. 1-Alkoxyethyl-3-hydroxypyridinium chlorides

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possess antielectrostatic properties, but are lacking antimicrobial activity. The antielectrostatic effect and antimicrobial activities are strongly dependent on the kind of substituent at the 3-position in the pyridine ring and are greatly affected by an alkoxy chain. Dimethylamino group in position three must be present for a high antielectrostatic and antimicrobial activity of the agent.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:325907 CAPLUS
DOCUMENT NUMBER: 137:201262
TITLE: *Synthesis* and antimicrobial activities of new pyridinium and benzimidazolium chlorides
AUTHOR(S): Pernak, Juliusz; Rogoza, Jarostaw; Mirska, Ilona
CORPORATE SOURCE: Poznan University of Technology, Poznan, 60-965, Pol.
SOURCE: European Journal of Medicinal Chemistry (2001), 36(4), 313-320
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:201262
IT 404965-60-2P 452281-20-8P 452281-21-9P
452281-22-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(*synthesis* and antibacterial and antifungal activities of new pyridinium and benzimidazolium chlorides)
RN 404965-60-2 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 24 in file .gra /

RN 452281-20-8 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 25 in file .gra /

RN 452281-21-9 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 26 in file .gra /

RN 452281-22-0 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 27 in file .gra /

IT 404965-58-8P 404965-59-9P 404965-71-5P
404965-72-6P 404965-84-0P 404965-85-1P

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404965-86-2P 404965-87-3P 404965-88-4P
404965-89-5P 404965-90-8P 404965-91-9P
404965-92-0P 404965-93-1P 452281-16-2P
452281-17-3P 452281-18-4P 452281-19-5P
452281-23-1P 452281-24-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)
(synthesis and antibacterial and antifungal activities of new
pyridinium and benzimidazolium chlorides)

RN 404965-58-8 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
chloride (9CI) (CA INDEX NAME)

/ Structure 28 in file .gra /

RN 404965-59-9 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 29 in file .gra /

RN 404965-71-5 CAPLUS

CN Pyridinium, 3,3'-(methylenediiimino)bis[1-[(nonyloxy)methyl]-, dichloride
(9CI) (CA INDEX NAME)

/ Structure 30 in file .gra /

RN 404965-72-6 CAPLUS

CN Pyridinium, 3,3'-(methylenediiimino)bis[1-(undecyloxy)methyl]-, dichloride
(9CI) (CA INDEX NAME)

/ Structure 31 in file .gra /

RN 404965-84-0 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
chloride (9CI) (CA INDEX NAME)

/ Structure 32 in file .gra /

RN 404965-85-1 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
chloride (9CI) (CA INDEX NAME)

/ Structure 33 in file .gra /

RN 404965-86-2 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 34 in file .gra /

RN 404965-87-3 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,

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chloride (9CI) (CA INDEX NAME)

/ Structure 35 in file .gra /

RN 404965-88-4 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 36 in file .gra /

RN 404965-89-5 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 37 in file .gra /

RN 404965-90-8 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 38 in file .gra /

RN 404965-91-9 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 39 in file .gra /

RN 404965-92-0 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 40 in file .gra /

RN 404965-93-1 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 41 in file .gra /

RN 452281-16-2 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(butoxymethyl)-, chloride (9CI) (CA INDEX NAME)

/ Structure 42 in file .gra /

RN 452281-17-3 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 43 in file .gra /

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RN 452281-18-4 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 44 in file .gra /

RN 452281-19-5 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 45 in file .gra /

RN 452281-23-1 CAPLUS
CN Pyridinium, 3,3'-(methylenediiimino)bis[1-[(decyloxy)methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 46 in file .gra /

RN 452281-24-2 CAPLUS
CN Pyridinium, 3,3'-(methylenediiimino)bis[1-[(dodecyloxy)methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 47 in file .gra /

GI

/ Structure 48 in file .gra /

AB Novel pyridinium, e.g I, and benzimidazolium, e.g. II, chlorides were obtained in high yield. The antimicrobial activities of three homologous series of pyridinium and benzimidazolium chlorides against cocci, rods, fungi and bacillus were measured. The antimicrobial activities of N,N'-bis[3-(1-alkoxymethyl)pyridinium chloride]methylenediamines, 1-undecyloxymethyl-3-(1-benzimidazolmethylamino)pyridinium, 1-undecyloxymethyl- and 1-dodecyloxymethyl-3-[1(benzotriazol-1-yl)methylamino]pyridinium chlorides exhibited strong activity and wide antibacterial spectra similar to the activity of benzalkonium chloride.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:773384 CAPLUS
DOCUMENT NUMBER: 136:263127
TITLE: Synthesis of 3-substituted pyridinium salts
AUTHOR(S): Pernak, Juliusz; Rogoza, Jaroslaw
CORPORATE SOURCE: Inst. Chem. Technol. Eng., Poznan Univ. Technol.,
Poznan, 60-965, Pol.
SOURCE: ARKIVOC [online computer file] (2000), 1(6), 889-904
CODEN: AKVCFI
URL: <http://www.arkat.org/arkat/journal/Issue6/ms06-0084.pdf>

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PUBLISHER: ARKAT Foundation
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
IT 404965-58-8P 404965-59-9P 404965-60-2P
404965-61-3P 404965-63-5P 404965-64-6P
404965-65-7P 404965-66-8P 404965-67-9P
404965-68-0P 404965-70-4P 404966-06-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of 3-substituted pyridinium salts)
RN 404965-58-8 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
chloride (9CI) (CA INDEX NAME)

/ Structure 49 in file .gra /

RN 404965-59-9 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 50 in file .gra /

RN 404965-60-2 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 51 in file .gra /

RN 404965-61-3 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
bromide (9CI) (CA INDEX NAME)

/ Structure 52 in file .gra /

RN 404965-63-5 CAPLUS
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
nitrate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4
CMF C22 H31 N4 O

/ Structure 53 in file .gra /

CM 2

CRN 14797-55-8
CMF N O3

/ Structure 54 in file .gra /

RN 404965-64-6 CAPLUS

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CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)méthyl]-,
iodide (9CI) (CA INDEX NAME)

/ Structure 55 in file .gra /

RN 404965-65-7 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4

CMF C22 H31 N4 O

/ Structure 56 in file .gra /

CM 2

CRN 14874-70-5

CMF B F4

CCI CCS

/ Structure 57 in file .gra /

RN 404965-66-8 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4

CMF C22 H31 N4 O

/ Structure 58 in file .gra /

CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

/ Structure 59 in file .gra /

RN 404965-67-9 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4

CMF C22 H31 N4 O

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/ Structure 60 in file .gra /

CM 2

CRN 14797-73-0

CMF Cl O4

/ Structure 61 in file .gra /

RN 404965-68-0 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, iodide (9CI) (CA INDEX NAME)

/ Structure 62 in file .gra /

RN 404965-70-4 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-69-1

CMF C26 H39 N4 O

/ Structure 63 in file .gra /

CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

/ Structure 64 in file .gra /

RN 404966-06-9 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-69-1

CMF C26 H39 N4 O

/ Structure 65 in file .gra /

CM 2

CRN 14797-73-0

CMF Cl O4

/ Structure 66 in file .gra /

10/717, 958

IT 404965-71-5P 404965-72-6P 404965-74-8P
404965-75-9P 404965-76-0P 404965-77-1P
404965-79-3P 404965-80-6P 404965-81-7P
404965-84-0P 404965-85-1P 404965-86-2P
404965-87-3P 404965-88-4P 404965-89-5P
404965-90-8P 404965-91-9P 404965-92-0P
404965-93-1P 404965-94-2P 404965-96-4P
404965-98-6P 404965-99-7P 404966-00-3P
404966-01-4P 404966-02-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3-substituted pyridinium salts)
RN 404965-71-5 CAPLUS
CN Pyridinium, 3,3'-(methylenediiimino)bis[1-[(nonyloxy)methyl]-, dichloride
(9CI) (CA INDEX NAME)

/ Structure 67 in file .gra /

RN 404965-72-6 CAPLUS
CN Pyridinium, 3,3'-(methylenediiimino)bis[1-(undecyloxy)methyl]-, dichloride
(9CI) (CA INDEX NAME)

/ Structure 68 in file .gra /

RN 404965-74-8 CAPLUS
CN Pyridinium, 3,3'-(methylenediiimino)bis[1-[(octyloxy)methyl]-,
diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-73-7
CMF C29 H50 N4 O2

/ Structure 69 in file .gra /

CM 2

CRN 14797-73-0
CMF Cl O4

/ Structure 70 in file .gra /

RN 404965-75-9 CAPLUS
CN Pyridinium, 3,3'-(methylenediiimino)bis[1-[(octyloxy)methyl]-, dibromate
(9CI) (CA INDEX NAME)

CM 1

CRN 404965-73-7
CMF C29 H50 N4 O2

/ Structure 71 in file .gra /

10/717,958

CM 2

CRN 15541-45-4
CMF Br O3

/ Structure 72 in file .gra /

RN 404965-76-0 CAPLUS
CN Pyridinium, 3,3'-(methylenediimino)bis[1-(octyloxy)methyl]-, diiodide
(9CI) (CA INDEX NAME)

/ Structure 73 in file .gra /

RN 404965-77-1 CAPLUS
CN Pyridinium, 3,3'-(methylenediimino)bis[1-(octyloxy)methyl]-, dibromide
(9CI) (CA INDEX NAME)

/ Structure 74 in file .gra /

RN 404965-79-3 CAPLUS
CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-,
bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 404965-78-2
CMF C37 H66 N4 O2

/ Structure 75 in file .gra /

CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS

/ Structure 76 in file .gra /

RN 404965-80-6 CAPLUS
CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-,
bis[(OC-6-11)-hexafluoroantimonate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 404965-78-2
CMF C37 H66 N4 O2

/ Structure 77 in file .gra /

CM 2

CRN 17111-95-4

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CMF F6 Sb
CCI CCS

/ Structure 78 in file .gra /

RN 404965-81-7 CAPLUS
CN Pyridinium, 3,3'-(methylenedimino)bis[1-(dodecyloxy)methyl]-, diiodide
(9CI) (CA INDEX NAME)

/ Structure 79 in file .gra /

RN 404965-84-0 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
chloride (9CI) (CA INDEX NAME)

/ Structure 80 in file .gra /

RN 404965-85-1 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
chloride (9CI) (CA INDEX NAME)

/ Structure 81 in file .gra /

RN 404965-86-2 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 82 in file .gra /

RN 404965-87-3 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 83 in file .gra /

RN 404965-88-4 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 84 in file .gra /

RN 404965-89-5 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

/ Structure 85 in file .gra /

RN 404965-90-8 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-,
chloride (9CI) (CA INDEX NAME)

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/ Structure 86 in file .gra /

RN 404965-91-9 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 87 in file .gra /

RN 404965-92-0 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 88 in file .gra /

RN 404965-93-1 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 89 in file .gra /

RN 404965-94-2 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-, iodide (9CI) (CA INDEX NAME)

/ Structure 90 in file .gra /

RN 404965-96-4 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-95-3
CMF C16 H20 N5 O

/ Structure 91 in file .gra /

CM 2

CRN 17111-95-4
CMF F6 Sb
CCI CCS

/ Structure 92 in file .gra /

RN 404965-98-6 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-97-5
CMF C17 H22 N5 O

10/717, 958

/ Structure 93 in file .gra /

CM 2

CRN 14797-73-0
CMF Cl O4

/ Structure 94 in file .gra /

RN 404965-99-7 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-, nitrate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-97-5
CMF C17 H22 N5 O

/ Structure 95 in file .gra /

CM 2

CRN 14797-55-8
CMF N O3

/ Structure 96 in file .gra /

RN 404966-00-3 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-95-3
CMF C16 H20 N5 O

/ Structure 97 in file .gra /

CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS

/ Structure 98 in file .gra /

RN 404966-01-4 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

10/717, 958

CM 1

CRN 404965-95-3
CMF C16 H20 N5 O

/ Structure 99 in file .gra /

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

/ Structure 100 in file .gra /

RN 404966-02-5 CAPLUS
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-, iodide (9CI) (CA INDEX NAME)

/ Structure 101 in file .gra /

AB A novel class of 3-substituted pyridinium salts have been synthesized in high yield by a convenient two-step procedure. A new synthetic pathway to 1-substituted benzimidazolium salts has been developed and the effects of the anionic component of the salts have been studied.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:614902 CAPLUS
DOCUMENT NUMBER: 111:214902
TITLE: α,ω -Di(phosphonomethyl) and α,ω -di(methylphosphinomethyl)
L- α,ω -diamino acids
AUTHOR(S): Nachev, I.
CORPORATE SOURCE: Res. Cent. "Konstrukcionni Polymeri", Sofia, 1528, Bulg.
SOURCE: Izvestiya po Khimiya (1988), 21(4), 477-83
CODEN: IZKHDX; ISSN: 0324-0401
DOCUMENT TYPE: Journal
LANGUAGE: Bulgarian
OTHER SOURCE(S): CASREACT 111:214902
IT 123529-71-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions with Et phosphite or methylphosphonite)
RN 123529-71-5 CAPLUS
CN Acetamide, N-[(acetyloxy)methyl]-N-[1-[(acetyloxy)methyl]-2-oxo-3-piperidinyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 102 in file .gra /

GI

10/717,958

/ Structure 103 in file .gra /

AB Treatment of the lactams of L-2,4-diaminobutanoic acid, L-ornithine, or L-lysine with HCHO in the presence 1,10-phenanthroline Co complex, followed by (CF₃CO)₂O in AcOH, afforded acetoxyethylated derivs. I (n = 1, 2, 3; R = AcOH). Condensation of the latter with P(OEt)₃ or MeP(OEt)₂ gave phosphorus derivs. I [R = R₁P(O)OEt, R₁ = OEt, Me]. Hydrolysis of the P ester groups with phosphodiesterase I and alkaline hydrolysis of the lactam ring and the acetyl group afforded title amino acids
HOPR₁(O)CH₂NHCH(CO₂)_{n+1}NHCH₂PR₁(O)OH.

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:542494 CAPLUS
DOCUMENT NUMBER: 89:142494
TITLE: Aging of soman-inhibited acetylcholinesterase:
inhibitors and accelerators
AUTHOR(S): Schoene, K.
CORPORATE SOURCE: Inst. Aerobiol., Fraunhofer-Ges., Schmallenberg-
Grafschaft, Fed. Rep. Ger.
SOURCE: Biochimica et Biophysica Acta (1978), 525(2), 468-71
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 61360-43-8 61368-95-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with soman-inhibited acetylcholinesterase, aging in
relation to)
RN 61360-43-8 CAPLUS
CN Pyridinium, 1,1'-[oxybis(methylene)]bis[3-[(aminocarbonyl)amino]-,
dichloride (9CI) (CA INDEX NAME)

/ Structure 104 in file .gra /

RN 61368-95-4 CAPLUS
CN Pyridinium, 1,1'-[oxybis(methylene)]bis[3-(acetylamino)-, dichloride (9CI)
(CA INDEX NAME)

/ Structure 105 in file .gra /

AB The influence of 27 possible effectors, mostly bispyridinium salts, on the dealkylation (aging) of soman-inhibited acetylcholinesterase was examined at pH 7.6 and 25°. In the absence of effectors, the rate constant of the aging process was 4.0 + 10⁻² min⁻¹. At 2 mM, the strongest inhibitor reduced the rate to 0.8 + 10⁻² min⁻¹, whereas it was raised to 8.2 + 10⁻² min⁻¹ by the most potent accelerator.

L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:402338 CAPLUS
DOCUMENT NUMBER: 73:2338
TITLE: Relation between chemical structure and cholinesterase
reactivating effect in a number of new asymmetric
bis-quaternary pyridinium salts. I. Derivatives of
4-hydroxyiminomethylpyridine
AUTHOR(S): Dirks, E.; Scherer, A.; Schmidt, Max; Zimmer, Gerhard
CORPORATE SOURCE: Battelle-Inst. e.V., Frankfurt/M., Fed. Rep. Ger.
SOURCE: Arzneimittel-Forschung (1970), 20(1), 55-62

10/717,958

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE:

Journal

LANGUAGE:

German

IT 27844-72-0 31984-53-9

RL: BIOL (Biological study)
(cholinesterase reactivation by)

RN 27844-72-0 CAPLUS

CN Pyridinium, 3-(dimethylamino)-1-[[[4-[(hydroxyimino)methyl]pyridinio]methoxy]methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 106 in file .gra /

RN 31984-53-9 CAPLUS

CN Pyridinium, 3-amino-4'-formyl-1,1'-(oxydimethylene)di-, dichloride, oxime (8CI) (CA INDEX NAME)

/ Structure 107 in file .gra /

AB Two series of asymmetric bis(pyridinium) salts, characterized by a methylene or O link joining the N atoms of the pyridine nuclei and having a p-aldoxime substituent on 1 of the pyridine nuclei were synthesized, including 1-[3-(3-dimethylamino-1-pyridinyl)propyl]-pyridine-4-aldoxime dibromide, 1-[3-(3-fluoro-1-pyridinyl)-2-oxapropyl]pyridine-4-aldoxime dichloride, 1-[3-(4-methoxy-1-pyridinyl)propyl]pyridine-4-aldoxime dibromide, and 1-[3-(4-tert-butyl-pyridinyl)-2-oxapropyl]pyridine-4-aldoxime dichloride. The ability of these compds. to reactivate acetylcholinesterase, previously inhibited by diisopropylfluorophosphate, as well as their inhibitory effect on untreated enzyme, depended on the radical added to the pyridine nuclei and on the nature of the bridge member. The size of the radical and its ability to dissociate into ions appear to be the essential factors, the electronic and phys. properties characterized by the Hammett σ -consts. and the Rf values being less important. The aldoxime radical had little effect on the activity of these compds., since it could be replaced by other radicals without affecting the results substantially. No significant relations between the increase in the hydrolysis rate of diisopropylfluorophosphate in the presence of bis(pyridinium) salts and their reactivating effect, or between the acute toxicity of the salts and their inhibitory effects on acetylcholine-esterase, were observed

L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:111249 CAPLUS

DOCUMENT NUMBER: 72:111249

TITLE: Relation between chemical structure and cholinesterase reactivating effect in new asymmetric pyridinium salts. II. Derivatives of 2-hydroxyiminomethylpyridine

AUTHOR(S): Dirks, E.; Scherer, A.; Schmidt, Max; Zimmer, Gerhard

CORPORATE SOURCE: Battelle-Inst. e. V., Frankfurt/M., Fed. Rep. Ger.

SOURCE: Arzneimittel-Forschung (1970), 20(2), 197-200

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: German

IT 27183-61-5P 27183-62-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27183-61-5 CAPLUS

CN Pyridinium, 3'-amino-2-formyl-1,1'-(oxydimethylene)di-, dichloride, oxime

10/717,958

(8CI) (CA INDEX NAME)

/ Structure 108 in file .gra /

RN 27183-62-6 CAPLUS
CN Pyridinium, 1-[[[3-(dimethylamino)pyridinio]methoxy]methyl]-2-[(hydroxyimino)methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 109 in file .gra /

GI For diagram(s), see printed CA Issue.
AB I (Q = CH₂ or O; R = m- or p-NO₂, MeSO₂, F, Cl, Br, I, SMe, NH₂, NMe₂, tert-Bu, MeO, CH₂:NOH, CO₂H, or CHN+Me₃; X = Cl or Br) were **prep'd** by authors' (1970) methods. I with R in the m-position did not reactivate acetylcholinesterase (EC. 3.1.1.7) inhibited with diisopropyl fluorophosphate. I (R = p-tert-Bu) showed significant reactivating activity at 1.05 e 10⁻² M. The reactivating activity of all I was lower than that of the corresponding p-aldoximes. I with large or polar R-substituents showed the lowest inhibiting activity on acetylcholinesterase. I (Q = O, R = m-substituent) showed the greatest inhibiting activity.

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